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Density functional theory calculations on azobenzene derivatives: a comparative study of functional group effect

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Abstract

© 2014, Springer-Verlag Berlin Heidelberg. Density functional theory (DFT) calculations have been used to investigate the structural properties, dipole moments, polarizabilities, Gibbs energies, hardness, electronegativity, HOMO/LUMO energies, and chemical potentials of trans and cis configurations of eight para-substituted azobenzene derivatives. All properties have been obtained using the B3LYP functional and 6-31++G(d,p) basis set. The planar structures have been obtained for all optimized trans configurations. The energy difference between trans and cis configurations for considered derivatives was found to be between 64.2–73.1 kJ/mole. It has been obtained that the p-aminodiazo-benzene (ADAB) has the difference in the dipole moments between trans and cis forms higher than for trans and cis azobenzene.

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Keywords

Azobenzene derivatives, cis-trans, Density functional theory, Dipole moment, Homo-Lumo, Polarizability